Coordinate Transformation Methods

Gérard Granet

GRATINGS: THEORY AND NUMERIC APPLICATIONS

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Chapter 8

Coordinate Transformation Methods

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8.1 Introduction

The C-method was born in the eighties in Clermont-Ferrand , France, from the need to solve rigorously diffraction problems at corrugated periodic surfaces in the resonance regime [1], [2], [3]. The main difficulty of such problems is the matching of boundaries conditions. It is obvious that any method aimed at solving Maxwell's equation is all the more efficient since it is able to fit the geometry of the problem. For that purpose, Chandezon et al introduced the so called translation coordinate system deduced from the Cartesian coordinate system $x,y,z)$ by the relations $x = x^1$, $y = x^2$, $z = x^3 + a(x^1)$ where $a(x^1)$ is a continuously differentiable function describing the surface profile. Hence since the boundary of the physical problem coincides with coordinate surfaces, writing boundary conditions is as simple as it is for classical problems in Cartesian, cylindrical, or spherical coordinates . This is the first ingredient of C-method. The second one is to write Maxwell's equation under the covariant form. This formulation comes from relativity where the use of curvilinear non orthogonal coordinate system is essential and natural. The main feature of this formalism is that Maxwell's equations remain invariant in any coordinate system, the geometry being shifted into the constitutive relations. Chandezon et al derived their 3D formulation from the general 4D relativistic Post's formalism [4] and evidently used tensorial calculus. Although it is with no doubt the most elegant and efficient way to deal with electromagnetic in general curvilinear coordinates it is also probably the reason why the theory appeared difficult to understand to many scientists. The third ingredient of C–method is that it is a modal method. This nice property is linked with the translation coordinate system in which a diffraction problem may be expressed as an eigenvalue eigenvector problem with periodic boundary conditions. The last feature of C-method is the numerical method of solution. The matrix operator is obtained by expanding field components into Floquet-Fourier harmonics and by projecting Maxwell's equations onto periodic exponential functions. The above four features may be resumed by saying that C-method is a curvilinear coordinate modal method by Fourier expansion [5]. Since the original papers, The C-method has gone through many stages of extension and improvement. The original theory was formulated for uncoated perfectly conducting gratings in classical mount. Various authors extended the method to conical diffraction mountings [6],[7]. Granet et al [11], Li et al [12] and Preist et al [13] allowed the various profiles

of a stack of gratings to be different from each other, although keeping the periodicity. Solving the vertical faces case in a simple manner, Plumey et al [14] have shown that the method can be applied to overhanging gratings Preist et al obtained the same results by applying the usual coordinate transformation to oblique coordinates [15]. In the numerical context, Li [16] and Cotter et al [17] improved the numerical stability of the C-method by using the S-matrix propagation algorithm for multilayer gratings. It is seen that C-method has been applied to a large class of surface relief gratings and multilayer coated gratings. The key point of C-method is the joint use of curvilinear coordinates and covariant formulation of Maxwell's equations. All the new developments in the modelling of gratings like Adaptive Spatial Resolution [18],[19],[20], and Matched coordinate [21]derive from this fundamental observation.

8.2 C-Method

In Euclidean space with origin O and basis vector $e_x, e_y, , e_z, ,$ let us consider an infinite cylindrical surface (Σ) whose elements are parallel to the y axis. This surface separates two linear homogeneous and isotropic media denoted (1) and (2). In Cartesian coordinates such a surface can be described by equation $z = a(x)$. Any electromagnetic field interacting with this particular geometry satisfies some boundary conditions. For instance, the tangential components of the electric field vector and the normal component of the displacement field vector are continuous at the surface. The point is that boundary conditions involve quantities that obviously depend on the position at which they are considered on the surface. We are thus led to look for a coordinate system which fits the problem and makes it more readily solvable than it is in a Cartesian framework. The so-called translation coordinate system (x^1, x^2, x^3) introduced by Chandezon and defined from the Cartesian coordinate system by the direct transformation (curvilinear coordinates to Cartesian coordinates) :

$$x = x^1, \qquad y = x^2, \qquad z = x^3 + a(x^1) \tag{8.1}$$

or the inverse transformation (Cartesian coordinates to curvilinear coordinates):

$$x^1 = x, \qquad x^2 = y, \qquad x^3 = z - a(x) \tag{8.2}$$

is one such system. It makes the surface (Σ) coincide with the coordinate surface $x^3 = 0$. A point $M(x, y, z = a(x)$ at the surface (Σ) is now referenced by the triplet $(x^1, x^2, 0)$. The coordinate surface $x^3 = x_0^3$ is obtained by translating each point at surface (Σ) with vector $x_0^3 e_z$, hence the name given by Chandezon to this particular coordinate system: translation coordinate system. The change of coordinates may also be considered as a change of variable. This view

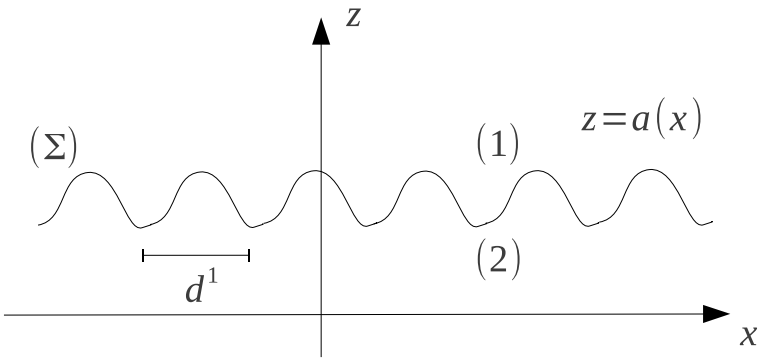

Figure 8.1: Geometry of the problem: Two media are separated by a cylindrical periodic surface, with period d^1 described by the equation z=a(x)

.

point allows a better understanding of the numerical behaviour of C-method and its connection with Rayleigh expansions. There is actually no difference in the way of deriving the elementary solutions of the scalar Helmholtz equation in Cartesian coordinates or in translation coordinate systems. Both are eigenvectors of an eigenvalue problem with pseudo-periodic boundary conditions. In both cases, the operator eigenvalue problem is transformed into a matrix eigenvalue problem thanks to the Galerkin method with pseudo periodic functions as expansion and test functions. Hence solving the scalar Helmholtz equation in any coordinate system is the very first step when implementing C-method. In the next paragraphs we shall focus on this issue before solving a grating problem.

8.2.1 Modal equation in the Cartesian coordinate system

Consider an homogeneous region with relative, possibly complex, permittivity, ε. In the harmonic regime with a time dependence of $\exp(-i\omega t)$, it is possible to construct general solutions to the field equations once we have general solutions to the scalar Helmholtz equation. So as a first task, we are going to investigate elementary solutions to the Helmholtz equation written in the translation coordinate system. Let us start from Cartesian coordinates in which 2D scalar Helmholtz equation is

$$\left(\partial_x^2 + \partial_z^2 + k^2\right) \mathscr{F} = 0 \tag{8.3}$$

where $k = \omega\sqrt{\mu_0\varepsilon}$ is the wave-number. The coefficients of the Helmholtz equation are independent of z so we seek solutions of the form $\mathscr{F}(x,z) = \exp(i\gamma z)F(x)$ The Helmholtz equation becomes:

$$(\partial_x^2 + k^2)F(x) = \gamma^2 F(x) \tag{8.4}$$

Function $F(x)$ is thus an eigenmode of equation (8.4). The requirement that the eigenmodes satisfy the pseudo-periodicity condition $F(x+d^1) = \exp(i\alpha_O d^1)F(x)$ is automatically fulfilled by their expansion into Floquet-Fourier series:

$$F(x) = \sum_{-\infty}^{+\infty} F_m \exp(i\alpha_m x) \tag{8.5}$$

$\alpha_m = \alpha_0 + mK_1$, $K_1 = \dfrac{2\pi}{d^1}$, $m \in \mathbb{N}$ and α_0 is some real parameter. By introducing (8.5) into (8.3) and by projecting onto pseudo-periodic functions $\exp(i\alpha_n x)$, one obtains the matrix equation:

$$\gamma^2 \boldsymbol{F} = \left[k^2 \boldsymbol{I} - \boldsymbol{\alpha}\right] \boldsymbol{F} \tag{8.6}$$

where $\boldsymbol{F}$ is a column vector whose elements are the F_m and $\boldsymbol{\alpha}$ is a diagonal matrix w hose elements are the α_m and $\boldsymbol{I}$ is the identity matrix. The solution to the above matrix eigenvalue equation is of course trivial since the matrix is diagonal. Let us introduce subscript q to number the eigenvalues and the eigenfunctions. The eigenvalues γ_q are deduced from their squared number:

$$\gamma_q^2 = k^2 - \alpha_q^2 \tag{8.7}$$

and the eigenvectors are determined by $F_{mq} = \delta_{mq}$ where δ_{mq} is the Kronecker symbol. The square root of γ_q^2 is defined as follows:

$$\gamma_q = \begin{cases} \sqrt{\gamma_q^2} & \text{if} \quad \gamma_q^2 \in \mathbb{R}^+ \\ \sqrt{-\gamma_q^2} & \text{if} \quad \gamma_q^2 \in \mathbb{R}^- \\ \left(\gamma_q^2\right)^{1/2} & \text{with positive imaginary part if} \quad \gamma_q^2 \in \mathbb{C} \end{cases} \tag{8.8}$$

Finally , $\mathscr{F}(x,z)$ can be represented by superposition of eigenmodes

$$\mathscr{F}(x,z) = \mathscr{F}^+(x,z) + \mathscr{F}^-(x,z) \tag{8.9}$$

with

$$\mathscr{F}^{+}(x,z) = \sum_{q=-\infty}^{q=+\infty} A_q^{+} \exp(i\gamma_q z) \sum_{m=-\infty}^{m=+\infty} \delta_{mq} \exp(i\alpha_m x) \tag{8.10}$$

$$\mathscr{F}^{-}(x,z) = \sum_{q=-\infty}^{q=+\infty} A_q^{-} \exp(-i\gamma_q z) \sum_{m=-\infty}^{m=+\infty} \delta_{mq} \exp(i\alpha_m x) \tag{8.11}$$

There are two sets of modes, the number of which are equal: those propagating or decaying in the positive direction of z and those propagating or decaying in the opposite direction. We denote these modes by superscript $+$ and $-$respectively. The z dependence of an eigenmode is determined by function $\exp(i\gamma_p z)$ By increasing z to $z+\Delta z$, $\exp(i\gamma_q z)$ is multiplied by $\exp(i\gamma_q \Delta z) = \exp(i\Re(\gamma_q)\Delta z) \times \exp(-\Im(\gamma_q)\Delta z)$ The real eigenvalues have $\Im(\gamma_q) = 0$ and correspond therefore to forward modes if $\Re(\gamma_q) > 0$ or backward modes if $\Re(\gamma_q) < 0$. The complex eigenvalues modes have a non-zero imaginary part and possibly also a non-zero real part. The associated eigenmodes decay forward if $\Im(\gamma_q) > 0$ or backward if $\Im(\gamma_q) > 0$. These expansions are known as Rayleigh expansions; they are linear combination of eigenvectors that we call hereafter Rayleigh eigenvectors R_q:

$$R_q(x) = \sum_{m=-\infty}^{m=+\infty} \delta_{mq} \exp(i\alpha_m x) \tag{8.12}$$

In Cartesian coordinates, the solutions to the Helmholtz equations may be regarded as the eigenvectors of a matrix equation. The eigenvalues γ_m are determined by the periodic lateral boundary conditions of the problem and are obtained analytically since the matrix is diagonal. The translation coordinate system preserves the z translation symmetry and also periodic lateral boundary conditions. We may then expect a great formal similitude between solutions obtained in each coordinate system.

8.2.2 Modal equation in terms of the new variables

In this section, we derive the master equation of C-method by considering the change of coordinates as a change of variables. For the change of variables $x^1 = x$, $x^2 = y$, $x^3 = z - a(x)$ the chain rule for derivatives has the form:

$$\begin{cases} \partial_x = \partial_1 - \dot{a}\partial_3 \\ \partial_y = \partial_2 \\ \partial_z = \partial_3 \end{cases} \tag{8.13}$$

Substituting the derivatives (8.13) into (8.3) gives:

$$\left((1+\dot{a}\dot{a})\partial_3^2 - \dot{a}\partial_1\partial_3 - \partial_1\dot{a}\partial_3 + \partial_1^2 + k^2\right)\mathscr{F}(x^1,x^3) = 0 \tag{8.14}$$

the solution of which are the same as the solutions of (8.13) expressed in terms of the new variables.

$$\begin{aligned} \mathscr{F}_a^{+}(x^1,x^3) &= \mathscr{F}^{+}(x = x^1, x^3 = z - a(x)) \\ &= \sum_{q=-\infty}^{q=+\infty} A_q^{+} \exp(i\gamma_q x^3) \sum_{m=-\infty}^{m=+\infty} \delta_{mq} \exp(i\gamma_q a(x^1)) \exp(i\alpha_m x^1) \end{aligned} \tag{8.15}$$

$$\begin{aligned}\mathscr{F}_a^-(x^1,x^3) &= \mathscr{F}^-(x=x^2,x^3=z-a(x)) \\ &= \sum_{q=-\infty}^{q=+\infty} A_q^- \exp(-i\gamma_q x^3) \sum_{m=-\infty}^{m=+\infty} \delta_{mq} \exp(-i\gamma_q a(x^1)) \exp(i\alpha_m x^1)\end{aligned} \tag{8.16}$$

The subscript a indicates the profile dependence of function $\mathscr{F}$.

We call function $\exp\left(\pm i\gamma_q a(x^1)\right)\exp\left(i\alpha_q x^1\right)$ the generalized Rayleigh eigenvector of order q. It is nothing more than plane wave $\exp(\pm i\gamma_q z)exp(i\alpha_q x^1)$ expressed in terms of the new variables x^1 and x^3 and is closely linked with function $a(x^1)$. Let us denote it $R_{a,q}^{\pm}$:

$$R_{a,q}^{\pm} = \exp\left(\pm i\gamma_q a(x^1)\right)\exp(i\alpha_q x^1) = \sum_{m=-\infty}^{m=+\infty} R_{amq}\exp(i\alpha_m x^1) \tag{8.17}$$

It is assumed so far that $a(x^1)$ is periodic with period d^1 hence:

$$\exp(\pm i\gamma_q a(x^1)) = \sum_{p=-\infty}^{p+\infty} L_p^{\pm}\exp\left(\frac{i2\pi p x^1}{d^1}\right) \tag{8.18}$$

with:

$$L_p^{\pm} = \frac{1}{d^1}\int_0^{d^1} \exp\left(\pm i\gamma_q a(x^1)\right)\exp\left(\frac{-i2\pi p x^1}{d^1}\right)dx^1 \tag{8.19}$$

In physical space, the generalized Rayleigh eigenvectors result from the product of a periodic function with a pseudo-periodic one. Thus, in Fourier space, the spectrum of the qth generalized Rayleigh eigenvector is obtained by translating the spectrum of function $\exp(\pm i\gamma_q z)$ with vector $2\pi q/d^1$, that is:

$$R_{amq}^{\pm} = L_{am-q}^{\pm} \tag{8.20}$$

Finally:

$$\mathscr{F}_a^+(x^1,x^3) = \sum_{q=-\infty}^{q=+\infty} A_q^+\exp(i\gamma_q x^3)\sum_{m=-\infty}^{m=+\infty} L_{am-q}^+\exp(i\alpha_m x^1) \tag{8.21}$$

$$\mathscr{F}_a^-(x^1,x^3) = \sum_{q=-\infty}^{q=+\infty} A_q^-\exp(-i\gamma_q x^3)\sum_{m=-\infty}^{m=+\infty} L_{am-q}^-\exp(i\alpha_m x^1) \tag{8.22}$$

Functions (8.21) and (8.22) give the general solution to (8.14). Indeed each element of this solution is a generalized Rayleigh eigenvector associated to index q such that $\gamma_q^2+\alpha_q^2=k^2$ and thus satisfies(8.14). The reason for that is obvious. It is obtain from (8.12) in which we have introduced the same change of variable as the one that has allowed us to get (8.14) from (8.3). From a practical view point, one can only manipulate finite size expansions and it does not make sense to speak of $R_{a,q}^{\pm}(x^1)$. That is why one may wonder if a generalized Rayleigh eigenvector is still a valid a solution of (8.14) when only a finite number of spatial Fourier harmonics is retained to represent it. Let us assume for a while the answer is yes and examine the involvements of such a claim. Introducing an integer M, hereafter denoted truncation number, and letting m run from $-M$ to M the truncated generalized Rayleigh eigenvector writes:

$$R_{a,q}^{\pm(M)}(x^1) = \sum_{m=-M}^{m=+M} R_{a,mq}^{\pm}\exp(i\alpha_m x^1) \tag{8.23}$$

Substituting ∂_3 with $i\gamma_q$, we have:

$$-(1+\dot{a}\dot{a})\gamma_q\dot{R}_a^{\pm(M)} - i(\dot{a}\partial_1+\partial_1\dot{a})\gamma_q R_a^{\pm,(M)} + (\partial_1^2+k^2)R_a^{\pm,(M)} = 0 \tag{8.24}$$

where $\dot{R}_a^{\pm(M)}$ denotes $\gamma_q R_a^{\pm,(M)}$. Replacing $\dot{a}$ by the coefficients of its Fourier series $\dot{a}_p$ and denoting $\dot{\boldsymbol{a}}$ the toeplitz matrix whose elements $\dot{a}_{mp}$ are the $\dot{a}_{m-p}$, it is easy to see that the matrix form of relation 8.24 is:

$$\begin{bmatrix} k^2\boldsymbol{I}-\boldsymbol{\alpha}^2 & 0 \\ 0 & \boldsymbol{I} \end{bmatrix} \begin{bmatrix} \boldsymbol{R}_{aq}^{\pm} \\ \dot{R}_{aq}^{\pm} \end{bmatrix} = \gamma_q \begin{bmatrix} -\dot{\boldsymbol{a}}\boldsymbol{\alpha}-\boldsymbol{\alpha}\dot{\boldsymbol{a}} & \boldsymbol{I}+\dot{\boldsymbol{a}}\dot{\boldsymbol{a}} \\ \boldsymbol{I} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{R}_{aq}^{\pm} \\ \dot{R}_{aq}^{\pm} \end{bmatrix} \tag{8.25}$$

where $\boldsymbol{R}_{aq}^{\pm}$ and $\dot{R}_{aq}^{\pm}$ are column vectors formed by the $2M+1$ Fourier coefficients of $R_{aq}^{\pm(M)}$ $\dot{R}_{aq}^{\pm(M)}$ respectively. (8.25) shows that γ_q and $\begin{bmatrix} \boldsymbol{R}_{aq}^{\pm} \\ \dot{R}_{aq}^{\pm} \end{bmatrix}$ are an eigenvalue and an eigenvector of the generalized matrix eigenequation $\boldsymbol{A}\psi = \rho\boldsymbol{B}\psi$. Since $R_{a,q}^{\pm}$ is an exact eigenvector of (8.14) its truncated part can only approximate the solution of (8.14) and consequently, mathematically speaking γ_q cannot be an eigenvalue of (8.25). It follows that our claim was false. Nevertheless, elementary pseudo-periodic solutions to (8.14) do exist and we will derive them in the next paragraph.

8.2.3 Fourier expansion of elementary waves in the translation coordinate system

In this paragraph, we derive the generalized eigenvalue eigenvector matrix equation starting from (8.14) the only assumption being the pseudo periodicity of the field and we discuss the obtained solutions. First, the propagation equation is rewritten as a pair of first-order equations:

$$\begin{bmatrix} k^2+\partial_1^2 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \mathscr{F} \\ \partial_3\mathscr{F} \end{bmatrix} = -\partial_3 \begin{bmatrix} \dot{a}\partial_1+\partial_1\dot{a} & 1+\dot{a}\dot{a} \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \mathscr{F} \\ \partial_3\mathscr{F} \end{bmatrix} \tag{8.26}$$

The coefficients of this equation do not depend on x^3 which allows to write the x^3 dependence as $\exp(i\rho x^3)$. The parameter ρ depends on the boundary conditions that $F(x^1,x^3)$ has to satisfy along x^1 direction. For gratings, periodic with period d^1 along x^1, $\mathscr{F}(x^1+d^1,x^3) = \exp(i\alpha_0 d^1)\mathscr{F}(x^1,x^3)$ where α_0 is some real parameter. $\partial_3\mathscr{F}$ verifies of course the same property. The above requirements on the solution are all fulfilled by expanding function $\mathscr{F}$ and $\partial_3\mathscr{F}$ under the form:

$$\mathscr{F}(x^1,x^3) = \exp(i\rho x^3)F_a(x^1) = \exp(i\rho x^3)\sum_{m=-M}^{m=M} F_{a,m}\exp(i\alpha_m x^1) \tag{8.27}$$

$$\partial_3\mathscr{F}(x^1,x^3) = \exp(i\rho x^3)\dot{F}_a(x^1) = \exp(i\rho x^3)\sum_{m=-M}^{m=M} \dot{F}_{a,m}\exp(i\alpha_m x^1) \tag{8.28}$$

Introducing the above expansions into (8.26) and projecting the latter onto $\exp\left(\dfrac{i2\pi n x^1}{d^1}\right)$ basis, we get the sought algebraic matrix eigenvalue equation from which eigenvalues ρ_q and eigenvectors $\boldsymbol{F}_{a,q}$ are readily obtained thanks to standard computer libraries:

$$\begin{bmatrix} k^2\boldsymbol{I}-\boldsymbol{\alpha}^2 & 0 \\ 0 & \boldsymbol{I} \end{bmatrix} \begin{bmatrix} \boldsymbol{F}_{a,q} \\ \dot{\boldsymbol{F}}_{a,q} \end{bmatrix} = \rho_{a,q} \begin{bmatrix} -\dot{\boldsymbol{a}}\boldsymbol{\alpha}-\boldsymbol{\alpha}\dot{\boldsymbol{a}} & \boldsymbol{I}+\dot{\boldsymbol{a}}\dot{\boldsymbol{a}} \\ \boldsymbol{I} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{F}_{a,q} \\ \dot{\boldsymbol{F}}_{a,q} \end{bmatrix} \tag{8.29}$$

As in the Cartesian coordinate system, it is observed numerically that there are two sets of modes, the number of which are equal: those propagating or decaying in the positive x^3 direction and those propagating or decaying in the opposite direction. Furthermore, it has been shown numerically and analytically [8], that, as the truncation number increases, the computed real eigenvalues converge to the real Rayleigh eigenvalues $\pm\gamma_q$.

$$\lim_{M\to\infty} \pm\rho_{a,q}^{M} = \pm\gamma_q^R \tag{8.30}$$

In the above relation, we have added an extra subscript M to indicate the truncation dependence. Indeed, the truncation order M has to be chosen large enough so that the computed real eigenvectors coincide with a great accuracy with their Rayleigh counterpart. In that case, provided that the eigenvalues are not degenerated, up to a multiplicative constant coefficient, the associated computed eigenvectors tend to the corresponding plane waves expressed in terms of the new variables (x^1, x^2, x^3).

$$\lim_{M\to\infty} F_{a,q}^{\pm(M)} = R_{a,q}^{\pm} \tag{8.31}$$

Thus in the translation coordinate system defined by $x^1 = x$, $x^2 = y$, $x^3 = z - a(x)$ as in the Cartesian coordinate system $Oxyz$, linear combinations of elementary solutions to the Helmholtz equation allow us to express electromagnetic field while giving it a physical meaning in terms of forward and backward waves.We write numerically the solution to the Helmholtz equation as:

$$\mathscr{F}_a^+(x^1,x^3) = \sum_{q\in U^+} A_q^+ \exp(i\rho_{a,q}^+ x^3) R_{a,q}^{+(M)}(x^1) + \sum_{q\in V^+} A_q^+ \exp(i\rho_{a,q}^+(x^3) F_{a,q}^+(x^1) \tag{8.32}$$

$$\mathscr{F}_a^-(x^1,x^3) = \sum_{q\in U^+} A_q^- \exp(i\rho_{a,q}^-(x^3) R_{a,q}^{-(M)}(x^1) + \sum_{q\in V^+} A_q^- \exp(i\rho_{a,q}^-(x^3) F_{a,q}^-(x^1) \tag{8.33}$$

with:

$$F_{a,q}^{\pm}(x^1) = \sum_{m=-M}^{m=+M} F_{a,mq}^{\pm} \exp(i\alpha_m x^1) \tag{8.34}$$

$U^{\pm}$, $V^{\pm}$ denote the sets of indices for the propagating and decaying orders in the positive and negative direction respectively.

$$U^+ = \left\{q/\Re(\rho_{a,q}) > 0 \text{ and } \Im(\rho_{a,q}) = 0\right\} \qquad U^- = \left\{q/\Re(\rho_{a,q}) < 0 \text{ and } \Im(\rho_{a,q}) = 0\right\} \tag{8.35}$$

$$V^+ = \left\{q/\Im(\rho_{a,q}) > 0\right\} \qquad V^- = \left\{q/\Im(\rho_{a,q}) < 0\right\} \tag{8.36}$$

8.3 Application to a grating problem

Let's come back to the one-dimensional grating problem. Consider the electromagnetic problem in which two homogeneous non magnetic media are separated by a cylindrical periodic surface with period d^1 which is invariant along the y axis in the Cartesian coordinate system $Oxyz$. Such a surface, described by equation $z = a(x)$ is illuminated from above by a unit amplitude linear polarized monochromatic plane wave with vacuum wavelength λ_0, angular frequency ω and vacuum wave number $k_0 = 2\pi/\lambda_0$. The wave vector is inclined at θ to the Oz axis. Medium (1)

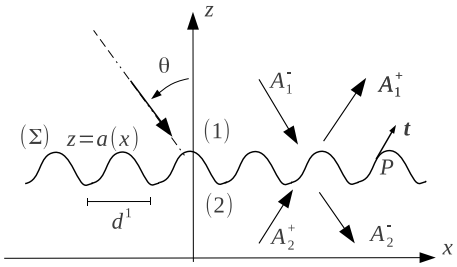

Figure 8.2: Geometry of the diffraction problem. Sketch of the coefficients for scattering matrix

and medium (2) have relative permittivity ε_1 and ε_2 respectively. Time dependence is expressed by the factor $\exp(-i\omega t)$ Such a problem is reduced to the study of the two fundamental cases of polarisation and the unknown function $\mathscr{F}(x,z)$ is the *y* component of the electric or the magnetic field for TE and TM polarization respectively. We solved half the problem since we already determined the general solution to the scalar Helmholtz equation as a linear combination of elementary waves the coefficients of which remain to calculate. The situation is very common in electromagnetic theory: the fields on both side of the grating are expanded in terms of the modes in the respective regions with unknown coefficients. A method of solution known as mode-matching method was developed in the context of guided waves in the micro-wave range. The grating may be considered as a generalized multi-port whose inputs are excited by waves that propagate or decay towards it giving rise to a response at the outputs that consists of the waves that propagate or decay away from it [25],[24]. The mode coupling is caused by the modulation of the interface and by the different constitutive parameters in either side of it. The so-called scattering matrix S_a defined as

$$\begin{bmatrix} \boldsymbol{A}^{(1)+} \\ \boldsymbol{A}^{(2)-} \end{bmatrix} = \boldsymbol{S}_a \begin{bmatrix} \boldsymbol{A}^{(1)-} \\ \boldsymbol{A}^{(2)+} \end{bmatrix} \tag{8.37}$$

provides a linear relation between the output and input coefficients. In a grating problem, the vector formed by the amplitudes of the incoming waves has only one non null component: that corresponding to the incident wave which was assumed enforced to one. The subscript a indicates that the S matrix depends on the profile function $a(x)$. We call $\boldsymbol{S}_a$ matrix an interface scattering matrix. The $\boldsymbol{S}_a$ matrix is derived from boundary conditions at the surface $x^3 = x_0^3$. The change of variable makes it easy to write them. We have solved the scalar Helmholtz equation, the scalar field being a field component tangent to the surface;indeed F coincides with H_y and E_y in TM polarisation and TE polarisation respectively. For simplicity, let us consider TE polarisation where the non null components of the electromagnetic field are E_y, H_x, H_z. Boundary conditions require matching the tangential components of the magnetic and electric field. We have already derived one of them, E_y, we have to derive the tangential component H_t of the electric field given by :

$$H_t = \boldsymbol{H}.\boldsymbol{t} \tag{8.38}$$

where $\boldsymbol{t}$ is the unit vector at point P which is tangential to the grating profile function. It is defined in terms of the $\boldsymbol{e}_x$ and $\boldsymbol{e}_z$ Cartesian unit vectors by:

$$\boldsymbol{t} = \frac{1}{\sqrt{1+\dot{a}^2}}(\boldsymbol{e}_x + \dot{a}\boldsymbol{e}_z) \tag{8.39}$$

The square root in the denominator represents a normalization factor that can be omitted since at a given point, it is identical on both sides of the boundary surface. let us introduce G such

that:

$$\mathscr{G} = iZ\boldsymbol{H}.\boldsymbol{t} \tag{8.40}$$

Where $Z = \sqrt{\mu_0/\varepsilon}$ is the wave impedance. From Maxwells equation we have $i\omega\mu_0 H_x = -\partial_z E_y$ and $i\omega\mu_0 H_z = \partial_x E_y$ thus :

$$\mathscr{G}(x,z) = -\frac{1}{k}(\partial_z \mathscr{F}(x,z) - \dot{a}\partial_x \mathscr{F}(x,z)) \tag{8.41}$$

substituting ∂_3 for ∂_z and $\partial_1 - \dot{a}\partial_3$ for ∂_x we get:

$$\mathscr{G}(x^1,x^3) = -\frac{1}{k}\left((1+\dot{a}\dot{a})\partial_3 - \dot{a}\partial_1\right)\mathscr{F}(x^1,x^3) \tag{8.42}$$

Similarly to $\mathscr{F}$, $\mathscr{G}$ depends on x^3 as $\exp(i\rho x^3)$ and we may write:

$$\mathscr{G}(x^1,x^3) = \exp(i\rho x^3)G(x^1) \tag{8.43}$$

We are now familiar with the operational rules that allow to associate in Fourier space a matrix with an operator. We have:

$$1 + \dot{a}\dot{a} \to \boldsymbol{I} + \dot{\boldsymbol{a}}\dot{\boldsymbol{a}}, \qquad \dot{a}\partial_1 \to i\dot{\boldsymbol{a}}\boldsymbol{\alpha} \tag{8.44}$$

From which we deduce:

$$ik\boldsymbol{G}_a^{\pm} = (I + \dot{\boldsymbol{a}}\dot{\boldsymbol{a}})\,\boldsymbol{F}_a^{\pm}\boldsymbol{\rho}_a - \dot{\boldsymbol{a}}\boldsymbol{\alpha}\boldsymbol{F}_a^{\pm} \tag{8.45}$$

where $\boldsymbol{\rho}$ is a diagonal matrix whose elements are the eigenvalues $\rho_{a,q}$. Writing the continuity of $\mathscr{F}^{(1)}$ and $\mathscr{F}^{(2)}$ and $\mathscr{G}^{(1)}/Z^{(1)}$ and $\mathscr{G}^{(2)}/Z^{(2)}$ at $x^3 = x_0^3$ is straightforward and leads to the following expression of the $\boldsymbol{S}_a$ matrix:

$$\boldsymbol{S}_a = \begin{bmatrix} \boldsymbol{F}_a^{(1)+} & -\boldsymbol{F}_a^{(2)-} \\ \boldsymbol{G}_a^{(1)+} & -\boldsymbol{G}_a^{(2)-} \end{bmatrix}^{-1} \begin{bmatrix} -\boldsymbol{F}_a^{(1)-} & \boldsymbol{F}_a^{(2)+} \\ -\boldsymbol{G}_a^{(1)-} & \boldsymbol{G}_a^{(2)+} \end{bmatrix} \tag{8.46}$$

The knowledge of $\boldsymbol{S}_a$ matrix allows to calculate the constant coefficients of outgoing waves. Since the spectrum of the solutions of the transformed Helmholtz equation include the generalized Rayleigh eigenvectors associated to real Rayleigh eigenvalues the efficiencies may be calculated in the very same way as in the Cartesian coordinate system.

$$R_q = |A_q^{(1)+}|^2 \frac{\gamma_q^{(1)}}{\gamma_0^{(1)}} \qquad T_p = |A_p^{(2)-}|^2 \frac{\gamma_p^{(2)}}{\gamma_0^{(1)}} \tag{8.47}$$

with:

$$\gamma_q^{(1)} = \sqrt{k_0^2\varepsilon_1 - \left(k_0\sqrt{\varepsilon}_1 \sin\theta + q\frac{2\pi}{d^1}\right)^2} \quad \gamma_p^{(2)} = \sqrt{k_0^2\varepsilon_2 - \left(k_0\sqrt{\varepsilon}_1 \sin\theta + p\frac{2\pi}{d^1}\right)^2} \tag{8.48}$$

The values of integers p and q are such that $\gamma_q^{(1)}$ and $\gamma_p^{(2)}$ are real.

8.3.1 Implementation of C-Method

The main interest to consider C-Method through a simple change of variable is to make us understand its numerical link with Rayleigh expansions and to calculate efficiencies as in the Cartesian Coordinate system. Within the framework of translation coordinate systems, starting from Maxwell's equations written under the covariant form, we have shown that all tangential components of the field at surface S could be generated from the longitudinal covariant components along the axis of invariance. Moreover,these components are solutions of the scalar Helmholtz equation. Therefore, one clearly understands that finding the elementary solutions of the scalar Helmholtz equation is the kernel of C-method. To summarize we may enunciate the different steps for solving a grating problem with C-method:

- Define a translation coordinate system.
- Find the elementary waves of the Helmholtz equation. For that purpose use the Galerkin method with $\exp(i\alpha_n x^1)$ as expansion and test functions. Substitute the generalized Rayleigh eigenvectors for the computed eigenvectors associated to real eigenvalues. Sort the elementary waves into forward and backward waves.
- Write boundary conditions at surface Σ and calculate efficiencies as in the Cartesian coordinate system.

8.4 Various formulations of C-method

So far, the Helmholtz equation in the translation coordinate system was derived by using the chain rule for derivatives in the Helmholtz equation written in the translation coordinate system. In this section,we start from the covariant Maxwell's equations and we show that they lead to several operators one of them being the propagation equation. In a homogeneous isotropic medium with permittivity ε and permeability μ, with a time dependence $\exp(-i\omega t)$,the symmetrized Maxwell equations write:

$$\begin{aligned} \xi^{\alpha\beta\gamma}\partial_\beta \mathscr{F}_\gamma &= k\sqrt{g}g^{\alpha\beta}\mathscr{G}_\alpha \\ \xi^{\alpha\beta\gamma}\partial_\beta \mathscr{G}_\gamma &= k\sqrt{g}g^{\alpha\beta}\mathscr{F}_\alpha \end{aligned} \tag{8.49}$$

where $k=\omega\sqrt{\mu\varepsilon}$, the $\mathscr{F}_\gamma$ and the $\mathscr{G}_\beta$ are the complex amplitudes of the electric field and of a renormalized magnetic field respectively. We restrict our analysis to 1D problems in which both the geometry and the solution are independent of y. Practically this means that ∂_2 is null as well as g^{12}, g^{21}, g^{32} and g^{23}. It follows that (8.49) decouple into two fully identical systems where the non null components are $\mathscr{F}_2$, $\mathscr{G}_1$, $\mathscr{G}_3$, and $\mathscr{G}_2$, $\mathscr{F}_1$, $\mathscr{F}_3$ respectively.The first set of three components corresponds to TE polarisation, the second one to TM polarisation. Both polarisations obey the same first order differential equations system written hereafter for TE polarisation:

$$-\partial_3 \mathscr{F}_2 = k\left(\sqrt{g}g^{11}\mathscr{G}_1 + \sqrt{g}g^{13}\mathscr{G}_3\right) \tag{8.50a}$$

$$\partial_1 \mathscr{F}_2 = k\left(\sqrt{g}g^{31}\mathscr{G}_1 + \sqrt{g}g^{33}\mathscr{G}_3\right) \tag{8.50b}$$

$$\partial_3 \mathscr{G}_1 - \partial_1 \mathscr{G}_3 = k\sqrt{g}g^{22}F_2 \tag{8.50c}$$

For TM polarisation, it is enough to permute $\mathscr{F}$ and $\mathscr{G}$. Among the three components of each system, two play a particular role. Let us assume that $x^3 = x_0^3$ separates two isotropic homogeneous media. Then, in TE polarisation $\mathscr{F}_2$ and $\mathscr{G}_1/\sqrt{\frac{\mu}{\varepsilon}}$ have to be continuous at surface $x^3 = x_0^3$. The same conclusions holds for $\mathscr{G}_2/\sqrt{\frac{\mu}{\varepsilon}}$ and $\mathscr{F}_1$ for TM polarisation. So, we have to solve (8.50) for the components labelled by two and by one. C-method is a Fourier based method which means that constitutive relations have to be written in Fourier space. In other words a matrix is to be associated to each element $\sqrt{g}g^{\alpha\beta}$ of the constitutive tensors. The way for doing so should follow the so-called "Fourier factorization" rules derived by Li [22],[23]. let us denote by $(\sqrt{g}g^{\alpha\beta})$ the matrix associated to coefficient $\sqrt{g}g^{\alpha\beta}$. According to Li's rules, the $(\sqrt{g}g^{\alpha\beta})$ write:

$$\begin{aligned}
(\sqrt{g}g^{11}) &= \left[\frac{1}{\sqrt{g}g^{11}}\right]^{-1} \\
(\sqrt{g}g^{13}) &= \left[\frac{1}{\sqrt{g}g^{11}}\right]^{-1}\left[\frac{g^{13}}{g^{11}}\right] \\
(\sqrt{g}g^{31}) &= \left[\frac{g^{31}}{g^{11}}\right]\left[\frac{1}{\sqrt{g}g^{11}}\right]^{-1} \\
(\sqrt{g}g^{33}) &= \left[\frac{1}{\sqrt{g}g^{11}}\right] + \left[\frac{g^{31}}{g^{11}}\right]\left[\frac{1}{\sqrt{g}g^{11}}\right]^{-1}\left[\frac{g^{13}}{g^{11}}\right] \\
(\sqrt{g}g^{22}) &= \left[\sqrt{g}g^{22}\right]
\end{aligned} \tag{8.51}$$

The notation $[f]$ designates the toeplitz matrix whose elements f_{mp} are the f_{m-p} elements of the Fourier series of function $f(x^1)$. For the translation coordinate (x^1, x^2, x^2) such that $x = x^1$, $y = x^2$, $z = x^3 + a(x^1)$, we have:

$$\begin{aligned}
\left(\sqrt{g}g^{11}\right) &\to \boldsymbol{I} \\
\left(\sqrt{g}g^{13}\right) &\to -\dot{\boldsymbol{a}} \\
\left(\sqrt{g}g^{31}\right) &\to -\dot{\boldsymbol{a}} \\
\left(\sqrt{g}g^{33}\right) &\to [\boldsymbol{I} + \dot{\boldsymbol{a}}\dot{\boldsymbol{a}}] \\
\left(\sqrt{g}g^{22}\right) &\to \boldsymbol{I}
\end{aligned} \tag{8.52}$$

In Fourier space, the derivative operator ∂_1 is associated to the diagonal matrix $i\boldsymbol{\alpha}$ the elements of which are the $i\alpha_m$ such that:

$$\alpha_m = \alpha_0 + m\frac{2\pi}{d^1} \tag{8.53}$$

Setting

$$\mathscr{F}_2(x^1, x^3) = \sum_{m=-M}^{m=+M} F_{2m}(x^3)\exp(i\alpha_m x^1) \tag{8.54a}$$

$$\mathscr{G}_1(x^1, x^3) = \sum_{m=-M}^{m=+M} G_{1m}(x^3)\exp(i\alpha_m x^1) \tag{8.54b}$$

$$\mathscr{G}_3(x^1, x^3) = \sum_{m=-M}^{m=+M} G_{3m}(x^3)\exp(i\alpha_m x^1) \tag{8.54c}$$

(8.54d)

We are now able to write (8.50) in Fourier space:

$$-\partial_3 \boldsymbol{F}_2 = k\left(\left(\sqrt{g}g^{11}\right)\boldsymbol{G}_1 + \left(\sqrt{g}g^{13}\right)\boldsymbol{G}_3\right) \tag{8.55a}$$

$$i\boldsymbol{\alpha}\boldsymbol{F}_2 = k\left(\left(\sqrt{g}g^{31}\right)\boldsymbol{G}_1 + \left(\sqrt{g}g^{33}\right)\boldsymbol{G}_3\right) \tag{8.55b}$$

$$\partial_3 \boldsymbol{G}_1 - i\boldsymbol{\alpha}\boldsymbol{G}_3 = k\left(\sqrt{g}g^{22}\right)\boldsymbol{F}_2 \tag{8.55c}$$

where $\boldsymbol{F}_2$, $\boldsymbol{G}_1$ $\boldsymbol{G}_3$ are column vectors of size $2M+1$ whose components are the $F_{2m}(x^3)$, $G_{1m}(x^3)$, $G_{3m}(x^3)$ respectively:

$$\boldsymbol{F}_2(x^3) = [F_{2,-M}(x^3),\, F_{2,-M+1}(x^3),\, \cdots, F_{2,0}(x^3),\, \cdots,\, F_{2,M-1}(x^3),\, F_{2,M}(x^3)]^T \tag{8.56a}$$

$$\boldsymbol{G}_1(x^3) = [G_{1,-M}(x^3),\, G_{1,-M+1}(x^3),\, \cdots,\, G_{1,0}(x^3),\, \cdots,\, G_{1,M-1}(x^3),\, G_{1,M}(x^3)]^T \tag{8.56b}$$

$$\boldsymbol{G}_3(x^3) = [G_{3,-M}(x^3),\, G_{3,-M+1}(x^3),\, \cdots G_{3,0}(x^3),\, \cdots,\, G_{3,M-1}(x^3),\, G_{3,M}(x^3)]^T \tag{8.56c}$$

where the exponent T is for the transposition.

8.4.1 Propagation equation in curvilinear coordinates

From Eqs (8.50a) and (8.50b), $\boldsymbol{G}_1$ and $\boldsymbol{G}_3$ may be expressed in terms of $\boldsymbol{F}_2$

$$k\boldsymbol{G}_1 = -\left(\sqrt{g}g^{33}\right)\partial_3 \boldsymbol{F}_2 + \left(\sqrt{g}g^{13}\right) i\boldsymbol{\alpha}\boldsymbol{F}_2 \tag{8.57}$$

$$k\boldsymbol{G}_3(x^3) = \left(\sqrt{g}g^{31}\right)\partial_3 \boldsymbol{F}_2(x^3) + \left(\sqrt{g}g^{11}\right) i\boldsymbol{\alpha}\boldsymbol{F}_2(x^3) \tag{8.58}$$

(8.50c), in which we substitute $\boldsymbol{G}_1$ and $\boldsymbol{G}_3$ with expressions (8.57) and (8.58), gives the propagation equation:

$$\left(-\boldsymbol{\alpha}\left(\sqrt{g}g^{11}\right)\boldsymbol{\alpha} + \partial_3\left(\sqrt{g}g^{33}\right)\partial_3 + i\boldsymbol{\alpha}\left(\sqrt{g}g^{13}\right)\partial_3 + \partial_3\left(\sqrt{g}g^{31}\right) i\boldsymbol{\alpha} + k^2\left(\sqrt{g}g^{22}\right)\right)\boldsymbol{F}_2(x^3) = 0 \tag{8.59}$$

which is rewritten as a pair of first-order differential equation as:

$$-i\partial_3 \boldsymbol{A}\begin{bmatrix}\boldsymbol{F}_2(x^3)\\ -i\partial_3\boldsymbol{F}_2(x^3)\end{bmatrix} = \boldsymbol{B}\begin{bmatrix}\boldsymbol{F}_2(x^3)\\ -i\partial_3\boldsymbol{F}_2(x^3)\end{bmatrix} \tag{8.60}$$

with:

$$\boldsymbol{A} = \begin{bmatrix}\boldsymbol{\alpha}\left(\sqrt{g}g^{13}\right) + \left(\sqrt{g}g^{13}\right)\boldsymbol{\alpha} & \left(\sqrt{g}g^{33}\right)\\ \boldsymbol{I} & \boldsymbol{0}\end{bmatrix} \tag{8.61}$$

$$\boldsymbol{B} = \begin{bmatrix}-\boldsymbol{\alpha}\left(\sqrt{g}g^{11}\right)\boldsymbol{\alpha} + k^2\left(\sqrt{g}g^{22}\right) & \boldsymbol{0}\\ \boldsymbol{0} & \boldsymbol{I}\end{bmatrix} \tag{8.62}$$

Since the coefficients of matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ are independent of variable x^3, we may seek vectors $\boldsymbol{F}_2(x^3)$, $\boldsymbol{G}_1(x^3)$,$\boldsymbol{G}_3(x^3)$ under the form:

$$\boldsymbol{F}_2(x^3) = \boldsymbol{F_2}\exp(i\rho x^3) \tag{8.63a}$$

$$-i\partial_3\boldsymbol{F}_2(x^3) = \dot{\boldsymbol{F}}_2\exp(i\rho x^3) \tag{8.63b}$$

$$\boldsymbol{G}_1(x^3) = \boldsymbol{G_1}\exp(i\rho x^3) \tag{8.63c}$$

$$\boldsymbol{G}_3(x^3) = \boldsymbol{G_3}\exp(i\rho x^3) \tag{8.63d}$$

This last step transforms (8.60) into a generalized eigenvalue eigenvector matrix equation:

$$\boldsymbol{A}\rho \begin{bmatrix} \boldsymbol{F}_2 \\ \dot{\boldsymbol{F}}_2 \end{bmatrix} = \boldsymbol{B} \begin{bmatrix} \boldsymbol{F}_2 \\ \dot{\boldsymbol{F}}_2 \end{bmatrix} \tag{8.64}$$

It is then easy to check that (8.64) is the same as (8.29). After $\boldsymbol{F}_2$ is determined, it remains to deduce $\boldsymbol{G}_1$ from (8.57).

8.4.2 "Classical" C-method operator

We call "classical" operator the operator derived by Chandezon in his early work. From (8.50b) and taking into account (8.63) we find an expression for $\boldsymbol{G}_3$ as follows:

$$\boldsymbol{G}_3 = \frac{1}{k}\left(\sqrt{g}g^{33}\right)^{-1} i\boldsymbol{\alpha}\boldsymbol{F}_2 - \left(\sqrt{g}g^{33}\right)^{-1}\left(\sqrt{g}g^{31}\right)\boldsymbol{G}_1 \tag{8.65}$$

Substituting $\boldsymbol{G}_3$ in (8.50a) and (8.50c) with the above expression yields:

$$\begin{bmatrix} -\left(\sqrt{g}g^{13}\right)\left(\sqrt{g}g^{33}\right)^{-1}\boldsymbol{\alpha} & ik\left(\left(\sqrt{g}g^{11}\right) - \left(\sqrt{g}g^{13}\right)\left(\sqrt{g}g^{33}\right)^{-1}\left(\sqrt{g}g^{31}\right)\right) \\ -ik\left(\left(\sqrt{g}g^{22}\right) - \frac{1}{k^2}\boldsymbol{\alpha}\left(\sqrt{g}g^{33}\right)^{-1}\boldsymbol{\alpha}\right) & -\boldsymbol{\alpha}\left(\sqrt{g}g^{33}\right)^{-1}\left(\sqrt{g}g^{31}\right) \end{bmatrix} \begin{bmatrix} \boldsymbol{F}_2 \\ \boldsymbol{G}_1 \end{bmatrix} = \rho \begin{bmatrix} \boldsymbol{F}_2 \\ \boldsymbol{G}_1 \end{bmatrix} \tag{8.66}$$

8.5 Multilayer grating

The extension of C-method to multilayer gratings is straightforward provided the interfaces which separate the layers share the same periodicity. It is just a generalization of the theory of planar stratified media. As a canonical case, let us consider a layer made of isotropic homogeneous media limited on the top by surface $z = a_j(x^1)$ and on the bottom by surface $z = a_{j+1}(x^1) = a_j(x^1) - t_j(x^1)$. When $t_j(x^1)$ is constant the two surfaces are parallel to each other. In homogeneous media the field is a superposition of forward and backward waves. The only places where coupling occurs are the interfaces. Thus, we have to describe two different phenomena: on the one hand scattering at the interfaces and on the other hand propagation or attenuation in the layer. To summarize we assimilate an interface to a $4N$-port local network ($N = 4M+1$, M being the truncation number) and a layer to a multi-channel pipe connecting the $2N$-ports of its input network and output network [24]. We have already defined interface scattering matrices which are local matrices in the sense they depend on the profile. In other words,in the context of C-method they depend on the coordinate system. Thus, for a layer bounded by two non parallel surfaces, we have to solve two eigenvalue problems for each surface which allows to calculate interface matrices $\boldsymbol{S}_{a_j}$ and $\boldsymbol{S}_{a_{j+1}}$. It remains to define and to calculate layer scattering matrices. Although two cases have to be considered according to whether the layer separates two identical surfaces or not, the line of reasoning is the same. As already mentioned, we have two coordinate systems such that $z = x_j^3 + a_j(x^1)$ and $z = x_{j+1}^3 + a_{j+1}(x^1)$. They are linked by the following relation:

$$x_j^3 = x_{j+1}^3 + a_{j+1}(x^1) - a_j(x^1) = x_{j+1}^3 - t_j(x^1) \tag{8.67}$$

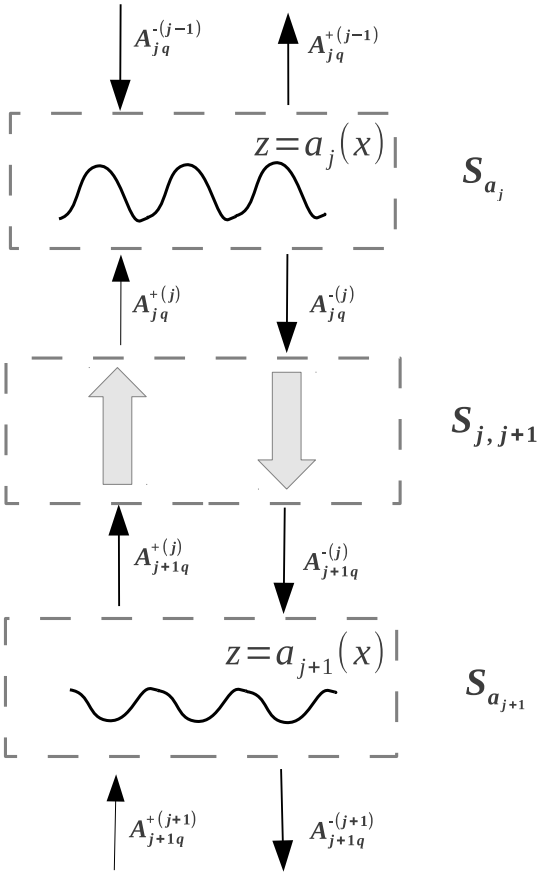

Figure 8.3: Schematic representation of diffraction at two surfaces separated by a layer

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In medium j, located in between surfaces $z = a_j(x^1)$ and $z = a_{j+1}(x^1)$, we may express the linear combination of forward and backard waves with coordinate $x_j^3 = 0$ as local origin (that is $z = a_j(x^1)$ and write:

$$\mathscr{F}_{a_j}^{(j)}(x_j^3, x^1) = \sum_q A_{j,q}^{(j)+} \exp(i\rho_{a_j,q}^{(j)+} x_j^3) F_{a_j,q}^{(j)+}(x^1) + \sum_q A_{j,q}^{(j)-} \exp(i\rho_{a_j,q}^{(j)-} x_j^3)) F_{a_j,q}^{(j)-}(x^1) \quad (8.68)$$

In the same medium j we may also choose $x_{j+1}^3 = 0$ as local origin (that is $z = a_{j+1}(x^1)$) which gives:

$$\mathscr{F}_{a_{j+1}}^{(j)}(x_{j+1}^3, x^1)) = \sum_q A_{j+1,q}^{(j)+} \exp(i\rho_{a_{j+1},q}^{(j)+} x_{j+1}^3) F_{a_{j+1},q}^{(j)+}(x^1) + \sum_q A_{j+1,q}^{(j)-} \exp(i\rho_{a_{j+1},q}^{(j)-}(x_{j+1}^3) F_{a_{j+1},q}^{(j)-}(x^1) \quad (8.69)$$

The layer is considered as a $4N - ports$ which connects input waves $\mathscr{F}_{a_j}^{(j)-}$ and $\mathscr{F}_{a_{j+1}}^{(j)+}$ to output waves $\mathscr{F}_{a_j}^{(j)+}$ and $\mathscr{F}_{a_{j+1}}^{(j)-}$, hence the definition of the layer S matrix:

$$\begin{bmatrix} A_{j,q}^{(j)+} \\ A_{j+1,q}^{(j)-} \end{bmatrix} = \boldsymbol{S}_{j,j+1} \begin{bmatrix} A_{j,q}^{(j)-} \\ A_{j+1,q}^{(j)+} \end{bmatrix} \quad (8.70)$$

At the input of the layer, that is at $x_j^3 = 0$, the outgoing waves correspond to the incoming wave of the output plane:

$$\mathscr{F}_{a_j}^{(j)+}(x_j^3 = 0) = \mathscr{F}_{a_{j+1}}^{(j)+}(x_{j+1}^3 = t_j(x^1)) \quad (8.71)$$

Similarly, at the output of the layer, that is $x^3_{j+1} = 0$, the outgoing waves correspond to the incoming waves of the input plane:

$$\mathscr{F}^{(j)-}_{a_{j+1}}(x^3_{j+1} = 0) = \mathscr{F}^{(j)-}_{a_j}(x^3_j = -t_j(x^1) \tag{8.72}$$

At this stage, we infer that layer S matrix looks like:

$$\boldsymbol{S}_{j,j+1} = \begin{bmatrix} 0 & \boldsymbol{P}^{(j)+} \\ \boldsymbol{P}^{(j)-} & 0 \end{bmatrix} \tag{8.73}$$

The sought sub-matrices $\boldsymbol{P}^{(j)+}$, $\boldsymbol{P}^{(j)-}$ depend on whether the layer faces are parallel or not.

8.5.1 Layer with non parallel faces

Consider equation (8.75) and write it in terms of the eigenvectors of both coordinate systems:

$$\sum_m \sum_q A^{(j)+}_{j,q} F^{(j)+}_{a_j,mq} exp(i\alpha_m x^1) = \sum_m \sum_q A^{(j)+}_{j+1,q} \exp(i\rho^+_{a_j+1,q} t_j(x^1)) F^{(j)+}_{a_{j+1},q} \exp(i\alpha_m x^1) \tag{8.74}$$

The left hand side purely consists of a linear combination of eigenvectors expanded onto the $\exp(i\alpha_m x^1)$ basis whereas the right hand side consists of a linear combination of eigenvectors each of which being multiplied by a periodic functions of the x^1 variable. In order to get a matrix relation between the $A^{(j)+}_{j,q}$ and the $A^{(j)+}_{j+1,q}$, we project (8.74) onto $\exp(i\alpha_m x^1)$. We get:

$$\sum_m \sum_q A^{(j)+}_{j,q} F^{(j)+}_{a_j,mq} = \sum_m \sum_q A^{(j)+}_{j+1,q} \tilde{F}^{(j)+}_{a_{j+1},q} \exp(i\alpha_m x^1) \tag{8.75}$$

with:

$$\tilde{F}^{(j)+}_{a_{j+1}mq} = \frac{1}{d^1} \int_0^{d^1} \left(\sum_l F^{(j)+}_{a_{j+1},lq} \exp(i\alpha_l x^1) \right) \exp(i\rho^{(j)+}_{a_j+1,q} t_j(x^1)) \exp(-i\alpha_m x^1) dx^1 \tag{8.76}$$

Then, the $\boldsymbol{P}^{(j)+}$ matrix is readily obtained as

$$\boldsymbol{P}^{(j)+} = \left(F^{(j)+}_{a_j} \right)^{-1} \tilde{\boldsymbol{F}}^{(j)+}_{a_{j+1}} \tag{8.77}$$

where $\boldsymbol{F}^{(j)+}_{a_j}$ (respectively $\tilde{\boldsymbol{F}}^{(j)+}_{a_{j+1}}$) is the matrix formed by juxtaposition of vectors $F^{(j)+}_{a_j,q}$ (respectively $\tilde{F}^{(j)+}_{a_{j+1}q}$. Similarly we have:

$$\sum_m \sum_q A^{(j)-}_{j+1,q} F^{(j)-}_{a_{j+1},mq} \exp(i\alpha_m x^1) = \sum_m \sum_q A^{(j)-}_{j,q} \exp(i\rho^{(j)-}_{a_j,q} t_j(x^1)) F^{(j)-}_{a_j,q} \exp(i\alpha_m x^1) \tag{8.78}$$

and

$$\sum_m \sum_q A^{-(j)}_{j+1,q} F^{(j)-}_{a_{j+1},mq} = \sum_m \sum_q A^{(j)-}_{j,q} \tilde{F}^{(j)-}_{a_j,q} \tag{8.79}$$

with:

$$\tilde{F}^{(j)-}_{a_jmq} = \frac{1}{d^1} \int_0^{d^1} \left(\sum_l F^{(j)-}_{a_j,lq} \exp(i\alpha_l x^1) \right) \exp(-i\rho^{(j)-}_{a_j+1,q} t_j(x^1)) \exp(-i\alpha_m x^1) dx^1 \tag{8.80}$$

from which we derive:

$$\boldsymbol{P}^{(j)-} = \left(F^{(j)-}_{a_{j+1}} \right)^{-1} \tilde{\boldsymbol{F}}^{(j)-}_{a_j} \tag{8.81}$$

8.5.2 Layer with parallel faces

In that case, the two coordinate systems are identical and $t_j(x^1)$ is a constant. Equations (8.72) and (8.75) reduce to:

$$\sum_m \sum_q A_{j,q}^{(j)+} F_{a_j,mq}^{(j)+} \exp(i\alpha_m x^1) = \sum_m \sum_q A_{j+1,q}^{+(j)} \exp(i\rho_{a_j,q}^{(j)+} t_j) F_{a_j,mq}^{(j)+} \exp(i\alpha_m x^1) \tag{8.82}$$

$$\sum_m \sum_q A_{j+1,q}^{(j)-} F_{a_j,q}^{(j)+} = \sum_m \sum_q A_{j,q}^{(j)-} \exp(-i\rho_{a_j,q}^{(j)-} t_j) F_{a_j,mq}^{(j)-} \exp(i\alpha_m x^1) \tag{8.83}$$

from which we easily deduce:

$$A_{j,q}^{(j)+} = A_{j+1,q}^{(j)+} \exp(i\rho_{a_j,q}^{(j)+} t_j) \text{ or } \boldsymbol{P}^{(j)+} = \text{diag}\left(\exp(i\rho_{a_j,q}^{(j)+} t_j)\right) \tag{8.84}$$

$$A_{j+1,q}^{(j)-} = A_{j,q}^{(j)-} \exp(-i\rho_{a_j,q}^{(j)-} t_j) \text{ or } \boldsymbol{P}^{(j)-} = \text{diag}\left(\exp(-i\rho_{a_j,q}^{(j)-} t_j)\right) \tag{8.85}$$

It should be noted that when $\rho_{a_j,q}^{(j)+}$ (respectively $\rho_{a_j,q}^{(j)-}$) is complex valued, its imaginary part is negative (respectively positive) . Since t_j is positive, exponential functions $\exp(\pm i\rho_{a_j,q}^{(j)\pm} t_j)$ associated to complex eigenvalues always decay when the layer thickness increases.

8.5.3 Combination of S matrices

The final step for analysing reflection and transmission by a layer is to combine the two interfaces S matrix and the layer S matrix. The tool for doing this is the Redheffer star product which gives the composition rules of two cascaded S matrices [26]. Consider two S matrices and partition them into four blocks:

$$\boldsymbol{S}_1 = \begin{bmatrix} \boldsymbol{S}_1^{11} & \boldsymbol{S}_1^{12} \\ \boldsymbol{S}_1^{21} & \boldsymbol{S}_1^{22} \end{bmatrix} \quad \boldsymbol{S}_2 = \begin{bmatrix} \boldsymbol{S}_2^{11} & \boldsymbol{S}_2^{12} \\ \boldsymbol{S}_2^{21} & \boldsymbol{S}_2^{22} \end{bmatrix} \tag{8.86}$$

The star product $*$ is defined by:

$$\boldsymbol{S} = \boldsymbol{S_1} * \boldsymbol{S_2} \tag{8.87}$$

$$\boldsymbol{S}^{11} = \boldsymbol{S}_1^{11} + \boldsymbol{S}_1^{12} \left(\boldsymbol{I} - \boldsymbol{S}_2^{11} \boldsymbol{S}_1^{22}\right)^{-1} \boldsymbol{S}_2^{11} \times \boldsymbol{S}_1^{21} \tag{8.88}$$

$$\boldsymbol{S}^{12} = \boldsymbol{S}_1^{12} \times \left(\boldsymbol{I} - \boldsymbol{S}_2^{11} \boldsymbol{S}_1^{22}\right)^{-1} \times \boldsymbol{S}_2^{12} \tag{8.89}$$

$$\boldsymbol{S}^{21} = \boldsymbol{S}_2^{21} \times \left(\boldsymbol{I} - \boldsymbol{S}_1^{22} \boldsymbol{S}_2^{11}\right)^{-1} \times \boldsymbol{S}_1^{21} \tag{8.90}$$

$$\boldsymbol{S}^{22} = \boldsymbol{S}_2^{22} + \boldsymbol{S}_2^{21} \times \left(\boldsymbol{I} - \boldsymbol{S}_1^{22} \boldsymbol{S}_2^{11}\right)^{-1} \times \boldsymbol{S}_1^{22} \times \boldsymbol{S}_2^{12} \tag{8.91}$$

where $\boldsymbol{I}$ is the identity matrix. The combined $\boldsymbol{S}$ matrix of the top and bottom interfaces and of the layer is given by:

$$\boldsymbol{S} = \boldsymbol{S}_{a_j} * \boldsymbol{S}_{j,j+1} * \boldsymbol{S}_{a_{j+1}} = \left(\boldsymbol{S}_{a_j} * \boldsymbol{S}_{j,j+1}\right) * \boldsymbol{S}_{a_{j+1}} = \boldsymbol{S}_{a_j} * \left(\boldsymbol{S}_{j,j+1} * \boldsymbol{S}_{a_{j+1}}\right) \tag{8.92}$$

and finally, it turns out that

$$\boldsymbol{S}^{11} = \boldsymbol{S}_{a_j}^{11} + \boldsymbol{S}_{a_j}^{12} \boldsymbol{P}(j)^{+} \boldsymbol{U}_2 \boldsymbol{P}^{(j)-} \boldsymbol{S}_{a_{j+1}}^{11} \tag{8.93}$$

$$\boldsymbol{S}^{12} = \boldsymbol{S}_{a_j}^{12} \boldsymbol{P}^{(j)+} \boldsymbol{U}_2 \boldsymbol{S}_{a_{j+1}}^{12} \tag{8.94}$$

$$\boldsymbol{S}^{21} = \boldsymbol{S}_{a_{j+1}}^{21} \boldsymbol{U}_1 \boldsymbol{P}^{(j)-} \boldsymbol{S}_{a_j}^{21} \tag{8.95}$$

$$\boldsymbol{S}^{22} = \boldsymbol{S}_{a_{j+1}}^{22} + \boldsymbol{S}_{a_{j+1}}^{21} \boldsymbol{P}^{(j)-} \boldsymbol{U}_1 \boldsymbol{P}^{(j)+} \boldsymbol{S}_{a_j}^{22} \tag{8.96}$$

where

$$\boldsymbol{U}_1 = \left(\boldsymbol{I} - \boldsymbol{S}_{a_j}^{22}\boldsymbol{P}^{(j)+}\boldsymbol{S}_{a_{j+1}}^{11}\boldsymbol{P}^{(j)-}\right)^{-1} \boldsymbol{U}_2 = \left(\boldsymbol{I} - \boldsymbol{S}_{a_{j+1}}^{11}\boldsymbol{P}^{(j)-}\boldsymbol{S}_{a_j}^{22}\boldsymbol{P}^{(j)+}\right)^{-1}$$

8.6 Extensions of C Method

The key idea of C-method as applied to diffraction by surface-relief gratings is to map the surface of the grating to a plane. Until now, we have only described profiles under the form $z = a(x)$. However, in Cartesian coordinates (x,y,z), a cylindrical surface whose generating line is parallel to the *Oy* axis may be described by the parametric equations:

$$x = f(x^1) \;\; z = g(x^1) \tag{8.97}$$

where f and g are two continuous functions. Now consider the following relations:

$$x = f(x^1) + c_1 x^3 \;\; y = x^2 \;\; z = g(x^1) + x^3 \tag{8.98}$$

where c_1 is a real constant. They define an additive change of coordinates whose metric tensor is given by:

$$g_{ij} = \begin{bmatrix} \partial_1^2 f + \partial_1^2 g & 0 & c_1\partial_1 f + \partial_1 g \\ 0 & 1 & 0 \\ c_1\partial_1 f + \partial_1 g & 0 & 1 + \partial_1^2 g \end{bmatrix} \tag{8.99}$$

Actually, the above matrix corresponds to a change of coordinates provided the Jacobian determinant J of the transformation does not go to zero.

$$J = \begin{vmatrix} \partial_1 x & \partial_3 x \\ \partial_1 z & \partial_3 z \end{vmatrix} = \begin{vmatrix} \partial_1 f & c_1 \\ \partial_1 g & 1 \end{vmatrix} = \partial_1 f - c_1\partial_1 g \tag{8.100}$$

More over, the metric tensor is independent of coordinate x^3 which means there exists a translation symmetry along x^3 axis. Hence Equations(8.98) define in a general way translation coordinate systems which allow to solve new classes of problems.

8.6.1 Oblique transformations

In Cartesian coordinates, usual coordinates lines of a plane are two straight lines orthogonal to each other. One can also imagine having straight lines which make an angle different from $\pi/2$. Consider the straight line Δ given by $z = \tan(\phi)x$ and let us call ϕ the obliquity angle. The following sets of relations define a coordinate system (x^1, x^3) in which lines parallel to Δ are coordinate lines $x^1 = constant$ and lines $x^3 =$ constant remain parallel to *Ox*

$$\begin{aligned} x &= x^1 + \frac{1}{\tan\phi} x^3 \\ z &= x^3 \end{aligned} \tag{8.101}$$

Such oblique transformation allow to model an extended class of surface shapes which would otherwise be numerically inefficient (very blazed gratings) or even impossible like overhanging gratings. As an illustrative example, consider in the coordinate system (x^1, x^3) the symmetric triangular function.

$$t(x^1) = \begin{cases} 2x^1 & 0 < x^1 < .5 \\ 2(1-x^1) & .5 < x^1 < 1 \\ 0 & \text{elsewhere} \end{cases} \tag{8.102}$$

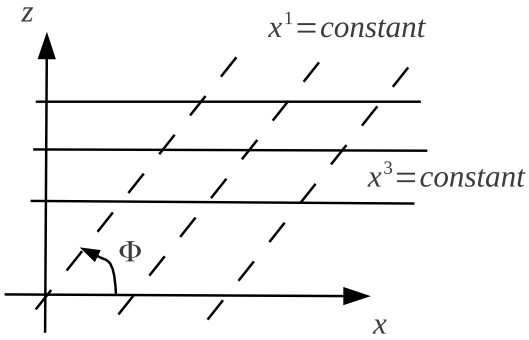


Figure 8.4: Coordinate system in which coordinate lines are parallel to Δ and to Ox axis

Using an oblique transformation one gets:

$$\begin{aligned} x &= x^1 + \frac{1}{\tan\phi}(x^3 + t(x^1)) \\ z &= x^3 + t(x^1) \end{aligned} \tag{8.103}$$

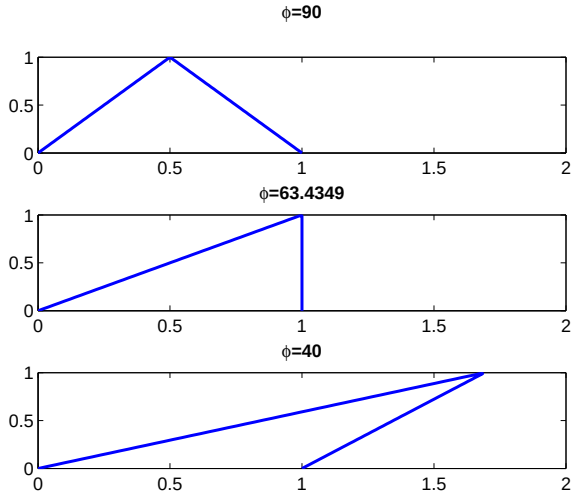


Figure 8.5: Echelette grating in three different oblique coordinate systems

Figure(8.5) shows three typical grating surfaces obtained with (8.103) and with $\phi = 90$, 63.4349 and 40 respectively, the latter demonstrating the extreme overhanging forms possible for small ϕ without the double value problem implicit with Cartesian coordinates.

8.6.2 Stretched coordinates

The essence of C-method is to choose a coordinate system that facilitate the solution of a given problem. Oblique transformations are a typical example of the usefulness of this technique. Indeed they provide an easy and elegant way to handle gratings with one vertical facet and also overhanging gratings. Similarly, we have believed for a long time that sharp edges were an intrinsic limitation of the C method. Actually, it turns out that transformations which stretch coordinates around the edges overcome the problem. With C-Method, the solution of Maxwell's equations is reduced to the solution of an algebraic eigenvalue problem in discrete Fourier

space. The derivation of the matrix operator involves two steps: (1) The electromagnetic field is expanded into Floquet–Fourier series, and (2) the derivative of the grating profile function is expanded into Fourier series. When the latter function is discontinuous, the Fourier method is known to converge slowly.This weakness remains even when the correct Fourier factorization of products of discontinuous periodic functions, as given by Li, is applied. The reason for slow convergence is that the spatial resolution of the Fourier expansion remains uniform within a grating period whatever the grating profile function may be. On the contrary, stretched coordinates allow a mapping of space that increases spatial resolution around the discontinuities of the derivative of the profile function. For this reason the technique is known as adaptive spatial resolution.

8.6.3 Parametric C-method

Whether for mandatory reasons as is the case for overhanging gratings or simply to improve convergence speed, the most general representation of a one dimensional profile happens to be a parametric one. Adding an additional degree of freedom with an obliquity angle, a class of translation coordinate systems has the form given by (8.98). Due to the translational symmetry along vector $\boldsymbol{e}_3 = c_1\boldsymbol{e}_x + \boldsymbol{e}_z$, a numerical solution in terms of eigenvectors and eigenvalues is possible. Equations (8.98) describe a coordinate system where coordinates lines $x^3 =$ constant coincide with functions which are periodic with period d^1 along direction Ox. Compared to the non-oblique coordinate system, the period d^1 and the direction of periodicity remain unaffected by the introduction of parameter c_1. Thus, assuming an incident plane wave vector $\boldsymbol{k}$ such that $\boldsymbol{k}.\boldsymbol{e}_x = \alpha_0$ the x^1 dependence is of the form $\exp(i\alpha_m x^1)$ with $\alpha_m = \alpha_0 + m\dfrac{2\pi}{d^1}$. So we have all the ingredients to determine the matrix from which eigenvectors and eigenvalues will be sought. In Fourier space, the matrices associated to the elements of the metric tensor are:

$$\begin{aligned}
\left(\sqrt{g}g^{11}\right) &= (c_1^2+1)\left[\dot{\boldsymbol{f}} - c_1\dot{\boldsymbol{g}}\right]^{-1} \\
\left(\sqrt{g}g^{13}\right) &= \left[\dot{\boldsymbol{f}} - c_1\dot{\boldsymbol{g}}\right]^{-1}\left[c_1\dot{\boldsymbol{f}} + \dot{\boldsymbol{g}}\right] \\
\left(\sqrt{g}g^{31}\right) &= \left[c_1\dot{\boldsymbol{f}} + \dot{\boldsymbol{g}}\right]\left[\dot{\boldsymbol{f}} - c_1\dot{\boldsymbol{g}}\right]^{-1} \\
\left(\sqrt{g}g^{33}\right) &= \left[\dot{\boldsymbol{f}} - c_1\dot{\boldsymbol{g}}\right] + (c_1^2+1)\left[c_1\dot{\boldsymbol{f}} + \dot{\boldsymbol{g}}\right]\left[\dot{\boldsymbol{f}} - c_1\dot{\boldsymbol{g}}\right]^{-1}\left[c_1\dot{\boldsymbol{f}} + \dot{\boldsymbol{g}}\right] \\
\left(\sqrt{g}g^{22}\right) &= \dot{\boldsymbol{f}} - c_1\dot{\boldsymbol{g}}
\end{aligned} \tag{8.104}$$

where $\dot{f}$ and $\dot{g}$ designates the toeplitz matrices formed by the elements of the Fourier series of $\partial_1 f$ and $\partial_1 g$ respectively.

8.6.4 Plane waves and parametric C-method

More over since the physics remains the same compared to non-oblique translation coordinate systems, eigenvectors separate into forward and backward waves as was already the case:

$$\mathscr{F}(x^1, x^3) = \sum_q A_q^{\pm} F_q^{\pm}(x^1) exp(i\rho_q^{\pm} x^3) \tag{8.105}$$

As in the classical translation coordinate system, we substitute the computed propagative forward and backward eigenvectors with the corresponding transformed plane waves . Consider

plane waves

$$\exp(i\alpha_n x)\exp(\pm i\gamma_n z)$$

such that $\pm\gamma_n \in R$. Taking into account (8.98),their expression in oblique coordinates is:

$$\exp\left(i(\alpha_n c_1 \pm \gamma_n)x^3\right)\exp\left(i(\alpha_n f(x^1) \pm \gamma_n g(x^1)\right) \tag{8.106}$$

hence the following correspondences between propagative waves in Cartesian coordinates and their computed counterparts in oblique coordinates:

$$\rho^{\pm,(M)}_{(p),n} \longleftrightarrow (\pm\gamma_n + \alpha_n c_1)\,; \quad F^{\pm}_{(p),n}(x^1) \longleftrightarrow \exp\left(i\alpha_n f(x^1) \pm i\gamma_n(g(x^1)\right) \tag{8.107}$$

We have added an extra subscript (p) and a superscript (M) to indicate that we only care about the above correspondence for propagative waves and that ρ depends on the truncation number.

8.6.5 Illustrative example

Consider a right angled triangular profile whose base is aligned on Ox. Other parameters are period d^1 and height h. It is illuminated by a plane wave inclined at θ to the Oz axis. In the context of C-method we ask ourselves which coordinate system choosing for modelling diffraction by such a grating. Here the main difficulty comes from the vertical facet located at $x = d^1$. The operator associated with C-method involves the derivative of the profile function. With a description of the profile by a function of the kind $z = a(x)$, the derivative is constant and everything happens as if the vertical did not exist. Should the vertical be replaced by a very sloping facet, then a highly located and large discontinuity in the derivative would appear. None of the situation is satisfactory. An easy way to overcome the problem consists in introducing an oblique coordinate system in which the vertical is transformed into a straight line with a "reasonable" slope. Actually, doing so amounts to parametrizing the profile in the Cartesian coordinate system.

8.6.5.1 Obliquity angle and parametrization of the profile

Since one of the facets of the grating is vertical, an inclined coordinate system is needed. On the one hand, the parameter c_1 is linked to the obliquity angle ϕ by $c_1 = 1/\tan\phi$ and on the other hand, according to (8.100) it should satisfy the constraint $1 - c_1\partial_x a > 0$. Hence, in principle ϕ may be any angle such that $\tan\phi < h/d$ Let t_1 be $\tan(\phi)$. On the first facet we have:

$$x = x^1 + \frac{1}{t_1}y, \qquad y = \frac{h}{d}x \tag{8.108}$$

and on the second one

$$x = d, \qquad d = x^1 + \frac{1}{t_1}y \tag{8.109}$$

Thus the parametrization of the profile is:

$$\begin{aligned} f(x^1) &= \frac{d}{d - t_1 h}x^1 \quad g(x^1) = \frac{h}{d - t_1 h}x^1 \quad \text{if } x^1 \leqslant x_0^1 \\ f(x^1) &= d \qquad\qquad\quad g(x^1) = \frac{1}{t_1}(x^1 - d) \quad \text{if } x^1 > x_0^1 \end{aligned} \tag{8.110}$$

with :

$$x_0^1 = d\left(1 - \frac{1}{t_1}\frac{h}{d}\right) \tag{8.111}$$

Now that we have parametrized the profile, it remains to define a translation direction. The direction which served to parametrize the profile is a natural choice although not mandatory. Once more, the only constraint is that the tangent of the chosen obliquity angle is smaller than h/d.

8.6.5.2 Stretched coordinates and parametrization of the profile

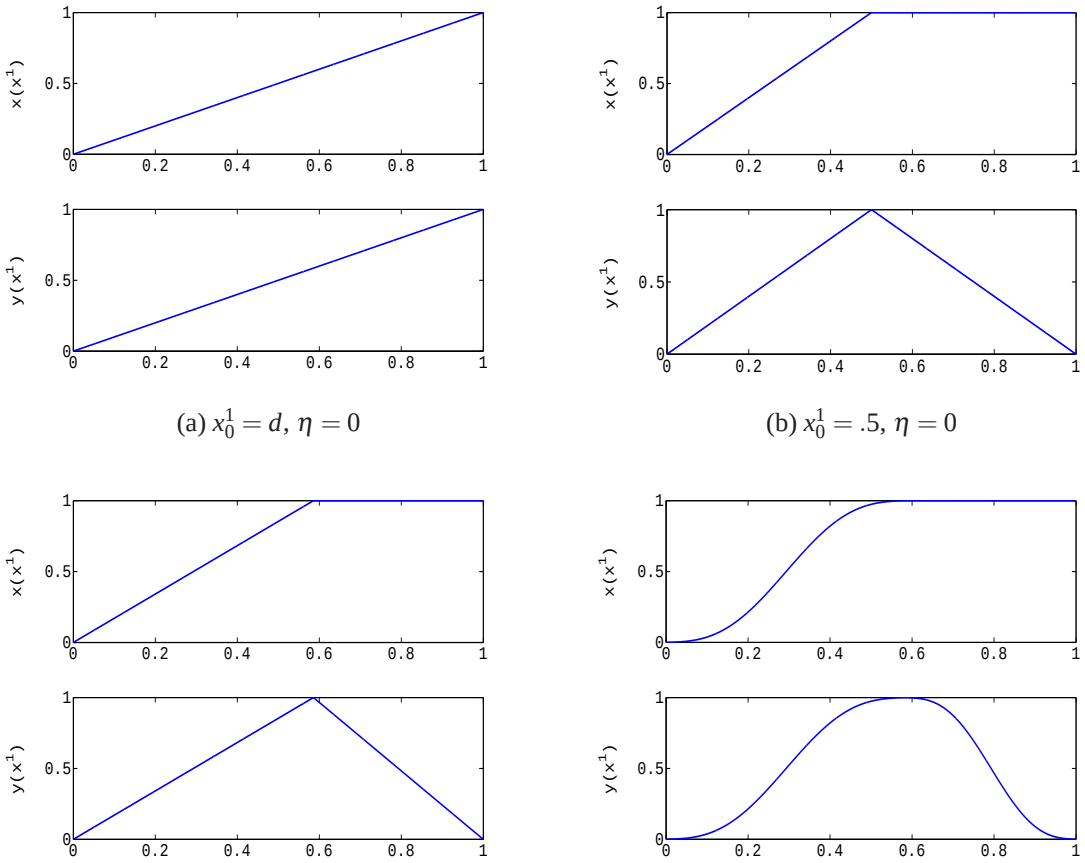
At $x^1 = 0$ and $x^1 = x_0^1$, the parametric functions $f(x^1)$ and $g(x^1)$ have jumps which can be reduced if one introduces an additional change of coordinates aimed at increasing spatial resolution around these points. Let x^1 be a function of a new variable u: $x^1 = s(u)$. The chain rule for derivative gives :

$$\partial_u x = \partial_1 f(x^1(s(u))\partial_u s, \qquad \partial_u y = \partial_1 g(x^1(s(u))\partial_u s \tag{8.112}$$

Compared to the initial parametrization, spatial resolution is modulated by the multiplicative factor $\partial_u s$. The smaller the latter, the higher the spatial resolution. A possible stretching function is as follows :

$$s(u) = \begin{cases} u - \dfrac{\eta x_0}{2\pi}\sin\left(\dfrac{2\pi u}{x_0}\right) & \text{if } 0 \leqslant u < x_0^1 \\ (u - x_0) - \dfrac{\eta(d^1 - x_0^1)}{2\pi}\sin\left(\dfrac{2\pi(u-x_0)}{d^1 - x_0^1}\right) & \text{if } x_0^1 \leqslant u < d^1 \end{cases} \tag{8.113}$$

The parameter η between zero and one controls the density of coordinate lines around the transition points. It allows to stretch space thinner where discontinuities of coefficients in Maxwell's equations occur. The larger η, the smaller $\partial_u s$ and thus the higher the spatial resolution. In principle the parameter η does not have to reach one because, in that case, the Jacobian would be zero. Figure (8.6) shows four possible parametrization of the considered right angle triangle. Case (a) corresponds to the usual representation $z = a(x)$.

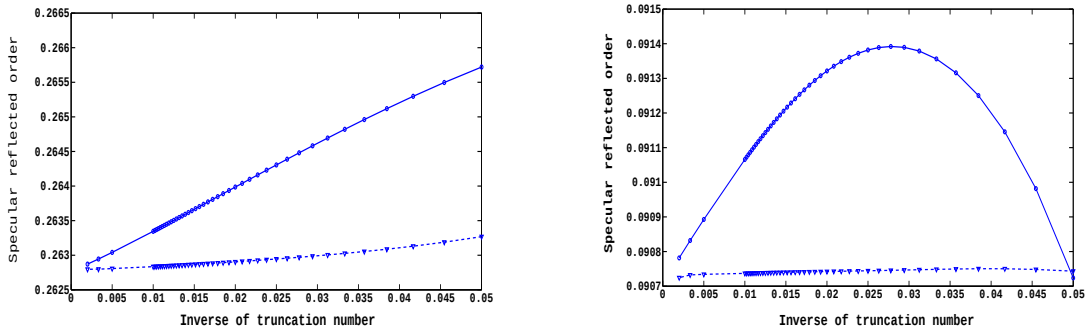


(a) $x_0^1 = d$, $\eta = 0$ (b) $x_0^1 = .5$, $\eta = 0$

(c) $x_0^1 = .5858$, $\eta = 0$ (d) $x_0^1 .5858$ $\eta = .95$

Figure 8.6: Various parametric representations of a right angle triangular profile

Finally, figure (8.7) shows the speed of convergence of the specular reflected order for a perfectly conducting right angle triangular profile for two different parametrizations. It has to be emphasized that modelling this kind of profile is out of reach for the "classical" C-method since it has a vertical facet.



(a) TE polarization, (b) TM polarization

Figure 8.7: Comparison of speed of convergence for two parametric representation of a right angle triangular profile. Full line: $x_0^1 = .5$, $\eta = 0$, dashed line: $x_0^1 = .4$, $\eta = .9$. Other parameters are: $\theta = 25°$, $\lambda = 1$,$h = d^1 = 1$

Appendix 8.A: Curvilinear Coordinates

In Cartesian coordinates we deal with three mutually perpendicular families of planes: x=constant, y=constant, z=constant. Imagine that we superimpose on this system three other families of surfaces. We may reference any variable point M by the intersection of three planes in Cartesian coordinates , ie by the triplet (x,y,z) or as the intersection of the three surfaces that form our new, curvilinear coordinates. Describing the curvilinear coordinates surfaces by $x^1 = constant$,$x^2 = constant$,$x^3 = constant$ we may identify our point by the triplet x,y,z as well as by x^1,x^2,x^3. This means that in principle we may define a curvilinear coordinate system from the Cartesian system (x,y,z) by:

$$x = x^{1'} = x^{1'}(x^1,x^2,x^3), y = x^{2'} = x^{2'}(x^1,x^2,x^3), z = \vec{x^3} = x^{3'}(x^1,x^2,x^3) \tag{8.114}$$

or by the inverse relations

$$x^1 = x^1(x^{1'},x^{2'},x^{3'}), x^2 = x^2(x^{1'},x^{2'},x^{3'}), x^3 = x^3(x^{1'},x^{2'},x^{3'}) \tag{8.115}$$

$x^{1'},x^{2'},x^{3'}$ respectively x^1,x^2,x^3 are regarded as independent and continuously differentiable functions of x^1, x^2 and x^3 respectively $x^{1'}$,$x^{2'}$,$x^{3'}$. let M denote a variable point referenced by the rectangular coordinates(x,y,z).At M the so-called natural referential$(M,\boldsymbol{e}_1,\boldsymbol{e}_2,\boldsymbol{e}_3)$is defined by the the following basis vectors:

$$\boldsymbol{e}_\alpha = \sum_{\beta'=1}^{\beta'=3} \frac{\partial x^{\beta'}}{\partial x^\alpha} \boldsymbol{e}_{\beta'} \tag{8.116}$$

with $e_{1'} = e_x$, $e_{2'} = e_y$, $e_{3'} = e_z$, e_x, e_y and e_z being the unit vectors of an orthogonal Cartesian referential. In a similar way we may write

$$\boldsymbol{e}_{\alpha'} = \sum_{\beta=1}^{\beta=3} \frac{\partial x^{\beta}}{\partial x^{\alpha'}} \boldsymbol{e}_{\beta} \tag{8.117}$$

Moreover introducing $\Lambda_\alpha^{\beta'} = \dfrac{\partial x^{\beta'}}{\partial x^\alpha}$ and Einsteins' summation convention Eq(8.116) and Eq(8.117) write:

$$\boldsymbol{e}_\alpha = \Lambda_\alpha^{\beta'} \boldsymbol{e}_{\beta'} \qquad \boldsymbol{e}_\alpha = \Lambda_\alpha^{\beta} \boldsymbol{e}_{\beta'} \tag{8.118}$$

vectors $\boldsymbol{e}_\alpha$ are tangent vectors along coordinate curve x^α. The matrix formed by the coefficient$\Lambda_\alpha^{\beta'}$ is the Jacobian matrix $\boldsymbol{J}$ of the change of coordinates. Since functions $x^{1'}$, $x^{2'}$,$x^{3'}$ are independent $\boldsymbol{J}$ is inverible and its inverse is formed by the coefficients $\Lambda_{\alpha'}^{\beta}$

$$\boldsymbol{J} = \begin{bmatrix} \Lambda_1^{1'} & \Lambda_1^{2'} & \Lambda_1^{3'} \\ \Lambda_2^{1'} & \Lambda_2^{2'} & \Lambda_2^{3'} \\ \Lambda_3^{1'} & \Lambda_3^{2'} & \Lambda_3^{3'} \end{bmatrix} \qquad \boldsymbol{J}^{-1} = \begin{bmatrix} \Lambda_{1'}^{1} & \Lambda_{1'}^{2} & \Lambda_{1'}^{3} \\ \Lambda_{2'}^{1} & \Lambda_{2'}^{2} & \Lambda_{2'}^{3} \\ \Lambda_{3'}^{1} & \Lambda_{3'}^{2} & \Lambda_{3'}^{3} \end{bmatrix} \tag{8.119}$$

One can also define basis vectors $\boldsymbol{e}^\alpha$ that are normal to coordinate surfaces $x^\alpha = \text{constant}$ by

$$\boldsymbol{e}^\alpha = \frac{\partial x^\alpha}{\partial x^{\alpha'}} \boldsymbol{e}^{\alpha'}, \qquad \text{with } \boldsymbol{e}^{\alpha'} = \boldsymbol{e}_{\alpha'} \tag{8.120}$$

The vectors $\boldsymbol{e}_\alpha$ and $\boldsymbol{e}^\beta$ form a set of reciprocal basis with $\boldsymbol{e}_\alpha.\boldsymbol{e}^\beta = \delta_\alpha^\beta$, where δ_α^β is the Kronecker delta. The representation of any vector $\boldsymbol{A}$ in one of these bases is:

$$\boldsymbol{A} = A^\alpha \boldsymbol{e}_\alpha = A_\alpha \boldsymbol{e}^\alpha \tag{8.121}$$

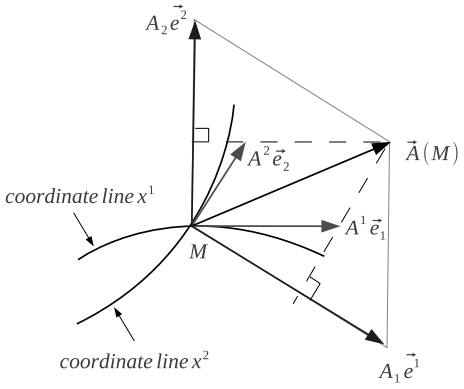


Figure 8.8: Curvilinear Coordinates:covariant and contravariant components of a vector in a plane

The A^α and the A_α are the contravariant components and the covariant components of vector $\boldsymbol{A}$ respectively. The nullity of a component of vector $\boldsymbol{A}$ may be geometrically interpreted as follows:
$A_\alpha = 0$: $\boldsymbol{A}$ is orthogonal to the tangent at point M to the coordinate line x^α
$A^\alpha = 0$: $\boldsymbol{A}$ belongs to the tangential plane at point M to coordinate surface x^α
In normalized orthogonal Cartesian coordinates differentiate contravariant and covariant components of a vector is generally not necessary. The Jacobian matrix allows to express the Cartesian components $A^{\alpha'} = A_{\alpha'}$ of vector $\boldsymbol{A}$ in terms of its local contravariant components $A^\alpha = \boldsymbol{A}.\boldsymbol{e}^\alpha$ or covariants components $A_\alpha = \boldsymbol{A}.\boldsymbol{e}_\alpha$:

$$A^{\alpha'} = A_{\alpha'} = \Lambda^{\alpha'}_{\alpha} A^\alpha \qquad \text{or} \qquad A^\alpha = \Lambda^{\alpha}_{\alpha'} A^{\alpha'} \tag{8.122}$$

$$A_{\alpha'} = \Lambda^{\alpha}_{\alpha'} A_\alpha \qquad \text{or} \qquad A_\alpha = \Lambda^{\alpha'}_{\alpha} A_{\alpha'} \tag{8.123}$$

The quantities

$$g_{\alpha\beta} = \boldsymbol{e}_\alpha.\boldsymbol{e}_\beta = \Lambda^{\alpha'}_{\alpha} \Lambda^{\beta'}_{\beta} g_{\alpha'\beta'} \tag{8.124}$$

define the metric of the coordinate system. In matrix form we have:

$$\left[g_{\alpha\beta}\right] = \boldsymbol{J}^t \boldsymbol{J} \tag{8.125}$$

and

$$g = \det(\left[g_{\alpha\beta}\right]) = \det(\boldsymbol{J})^2 = \det\left(\Lambda^{\alpha'}_{\beta}\right) \tag{8.126}$$

The $g_{\alpha\beta}$ establish a connexion between the A^α and the A_β

$$A_\alpha = \boldsymbol{e}_\alpha.\left(A^\beta.\boldsymbol{e}_\beta\right) = g_{\alpha\beta} A^\beta \qquad \text{or} \qquad A^\beta = g^{\beta\alpha} A_\alpha \tag{8.127}$$

Appendix 8.B: Transformation of Maxwell's equations

We have seen that the natural referentiel gives the tools to easily maipulate tangential and normal components of a vector field.Therefore, writting boundary conditions at a surface should be

straightforward. We need now to express Maxwell's equation in the new coordinate system. For that purpose, we may follow a tensorial approach or stay at an elementary level and make a simple change of coordinates and components in the usual Maxwell's equations. We present briefly both points of view. A time dependence of the form $\exp(-i\omega t)$ is assumed.

Vectorial approch

Let us start from one of the Maxwell's curl equation written in the Cartesian coordinate system and in an homogeneous medium with permittivity ε and permeability μ

$$\xi^{\alpha'\beta'\gamma'}\partial_{\beta'}H_{\gamma'} = -i\omega\varepsilon E_{\alpha'} \tag{8.128}$$

where $\xi^{\alpha'\beta'\gamma'}$ stands for the Levi-Civita indicator :

$$\xi^{\alpha'\beta'\gamma'} = \begin{cases} 1 \text{ for } \alpha'\beta'\gamma' = 123, 231, 312 \\ -1 \text{ for } \alpha'\beta'\gamma' = 321, 213, 132 \\ 0 \text{ otherwise} \end{cases} \tag{8.129}$$

Then let us change the coordinates: $\partial_{\beta'} = \Lambda^{\alpha}_{\beta'}\partial_{\alpha}$ and the components $H_{\gamma'} = \Lambda^{\beta}_{\gamma'}H_{\beta}$

$$\xi^{\alpha'\beta'\gamma'}\Lambda^{\alpha}_{\beta'}\partial_{\alpha}\left(\Lambda^{\beta}_{\gamma'}H_{\beta}\right) = -i\omega\varepsilon E_{\alpha'} \tag{8.130}$$

The left hand side of the above equation is equal to:

$$\xi^{\alpha'\beta'\gamma'}\Lambda^{\alpha}_{\beta'}\left(\Lambda^{\beta}_{\gamma'}\partial_{\alpha}H_{\beta}\right) + \xi^{\alpha'\beta'\gamma'}\Lambda^{\alpha}_{\beta'}\left(\partial_{\alpha}\Lambda^{\beta}_{\gamma'}\right)H_{\beta} \tag{8.131}$$

on the one hand we have

$$\Lambda^{\alpha}_{\beta'}\partial_{\alpha}\Lambda^{\beta}_{\gamma'} = \partial_{\beta'}\Lambda^{\beta}_{\gamma'} \tag{8.132}$$

and the other hand this term is symmetrical with respect to β' and γ'. Thus by applying the operator $\xi^{\alpha'\beta'\gamma'}$ which is antisymmetric with respect to β' and γ' we obtain 0. Thus, the Maxwell curl equation reduces to:

$$\xi^{\alpha'\beta'\gamma'}\Lambda^{\alpha}_{\beta'}\Lambda^{\beta}_{\gamma'}\partial_{\alpha}H_{\beta} = -i\omega\varepsilon E_{\alpha'} \tag{8.133}$$

let us multiply both sides by $\Lambda^{\gamma}_{\alpha'}$ and make summation on dummy index α'. We obtain:

$$\xi^{\gamma\alpha\beta}\det\left(\Lambda^{\alpha}_{\beta'}\right)\partial_{\alpha}H_{\beta} = -i\omega\varepsilon\Lambda^{\gamma}_{\alpha'}E^{\alpha'} = -i\omega\varepsilon E^{\gamma} = -i\omega\varepsilon g^{\gamma\beta}E_{\beta} \tag{8.134}$$

Finally we get:

$$\xi^{\gamma\alpha\beta}\partial_{\alpha}H_{\beta} = -i\omega\varepsilon\sqrt{g}g^{\gamma\beta}E_{\beta} \tag{8.135}$$

and

$$\xi^{\gamma\alpha\beta}\partial_{\alpha}E_{\beta} = i\omega\mu\sqrt{g}g^{\gamma\beta}H_{\beta} \tag{8.136}$$

setting

$$\mathscr{F}_{\alpha} = E_{\alpha} \qquad \mathscr{G}_{\alpha} = iZH_{\alpha} \qquad \text{with } Z = \sqrt{\frac{\mu}{\varepsilon}} \tag{8.137}$$

we then obtain a set of equations relating the complex amplitudes of the field components where the $\mathscr{F}_{\alpha}$ and the $\mathscr{G}_{\alpha}$ play a fully symmetric role:

$$\begin{aligned} \xi^{\alpha\beta\gamma}\partial_{\beta}\mathscr{F}_{\gamma} &= k\sqrt{g}g^{\alpha\beta}\mathscr{G}_{\alpha} \\ \xi^{\alpha\beta\gamma}\partial_{\beta}\mathscr{G}_{\gamma} &= k\sqrt{g}g^{\alpha\beta}\mathscr{F}_{\alpha} \end{aligned} \tag{8.138}$$

where $k = \omega\sqrt{\mu\varepsilon}$

Appendix 8.C: Summary of tensorial approach

In curvilinear coodinates systems, the Maxwell's equations are based on the tensorial formalism deduced from relativity. If we consider only materials which are stationary with respect to the coordinate system, then the four-dimensional formalism developed by Post can be simplified. Maxwell equations are written :

$$\begin{array}{l} \xi^{\alpha\beta\gamma}\partial_\beta E_\gamma = -\partial_t B^\alpha \\ \xi^{\alpha\beta\gamma}\partial_\beta H_\gamma = \partial_t D^\alpha + J^\alpha \\ \partial_\alpha D^\alpha = \rho \\ \partial_\alpha B^\alpha = 0 \end{array} \tag{8.139}$$

Post's formalism preserves the affine nature of Maxwell' equations: their expression is independent of the coordinate system. The geometry only appears in the constitutive equations along with the material's properties

$$D^\alpha = \varepsilon^{\alpha\beta} E_\beta \qquad B^\alpha = \mu^{\alpha\beta} H_\beta \tag{8.140}$$

In a perfectly linear, isotropic media with permittivity ε and μ, these relation ships become:

$$\varepsilon^{\alpha\beta} = \varepsilon\sqrt{g}g^{\alpha\beta} \qquad \varepsilon^{\alpha\beta} = \varepsilon\sqrt{g}g^{\alpha\beta} \tag{8.141}$$

where $g^{\alpha\beta}$ are the contravariant components of the metric tensor.

$$\left(g^{\alpha\beta}\right) = \left(g_{\alpha\beta}\right)^{-1} \qquad g = (det)(g_{\alpha\beta}) \tag{8.142}$$

In an arbitrary curvilinear coordinates systeme x^α, if the surface separating two materials, denoted (1) and (2), coincides with a surface of coordinates $x^3 = constant$, for example, then the conditions of continuity are expressed quite simply

$$\text{tangential component continuity: } \begin{cases} a_1(1) = a_1(2) \\ a_2(1) = a_2(2) \end{cases} \tag{8.143}$$

$$\text{normal component continuity: } a^3(1) = a^3(2) \tag{8.144}$$

Assuming a time dependence of the form $\exp(-i\omega t)$, in a source free region if we substitute the constitutive equations for the material8.141 into Maxwell equations in the covariant form 8.139, setting

$$\mathscr{F}_\alpha = E_\alpha \qquad \mathscr{G}_\alpha = -iZH_\alpha \qquad \text{with } Z = \sqrt{\frac{\mu}{\varepsilon}} \tag{8.145}$$

we then obtain a set of equations relating the complex amplitudes of the field components where the $\mathscr{F}_\alpha$ and the $\mathscr{G}_\alpha$ play a fully symmetric role:

$$\begin{array}{l} \xi^{\alpha\beta\gamma}\partial_\beta \mathscr{F}_\gamma = k\sqrt{g}g^{\alpha\beta}\mathscr{G}_\alpha \\ \xi^{\alpha\beta\gamma}\partial_\beta \mathscr{G}_\gamma = k\sqrt{g}g^{\alpha\beta}\mathscr{F}_\alpha \end{array} \tag{8.146}$$

where $k = \omega\sqrt{\mu\varepsilon}$

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